# DICE: Database for the International Handbook of Evaluated Criticality Safety Benchmark Experiments

**Users' Manual** 

**Version: September 2003** 

What is DICE	3
Requirements and compatibilityInstallation	
Troubleshooting	4
Screen resolution	5
Using DICE	6
General overview	6
Search screen	6
Results screen	7
Summary table	8
Plotting capabilities	
How to plot neutron spectra	
Changing the energy structure	
Choosing the type of representation	
How to plot sensitivity coefficients	14
Search themes	16
Example of a free text field selection	
Example of a selection in a selection list	
Example of a selection in range of real values	
Example of a selection in a combination of selection list and range of real values	
Example of a selection in a range of integer values	22
Local and remote databases	22
Live update	23
Settings	23
Contributors	25

## What is DICE

The "International Handbook of Evaluated Criticality Safety Benchmark Experiments" is a collection of evaluated experimental data representative of configurations encountered in the nuclear fuel cycle. The data is useful for the validation of neutronic codes and associated nuclear data libraries used for criticality-safety analysis.

The handbook is produced in electronic format (pdf files) where the experiments are grouped into evaluations, categorized by fissile media (Pu, Low Enriched Uranium...), fuel form (Solution, Metal...) and by neutron spectrum description (Thermal, Fast...). The evaluations are structured into different sections where the experimental program is described, the data are evaluated, the effect of experimental data uncertainties is assessed and benchmark models are described. Sample calculations are also presented and calculated spectral characteristics of the experiments given.

DICE is a tool intended to make more efficient use of the handbook. Two objectives were assigned to DICE:

- Provide a summary description of each experimental configuration, where the main characteristics of the experiments are displayed in a concise uniform format.
- Allow users to search the handbook for experimental configurations that satisfy their desired input criteria.

To meet these objectives, a relational database was created. Selected information from each evaluation in the handbook was entered into the database in order to provide the data required for the summaries or specific searches. A user interface was then developed to query the database and to generate different output formats (tables, summary pages, plots).

## Requirements and compatibility

The minimum requirements for running DICE are:

- A Java virtual machine installed on the computer (see the next paragraph).
- An Acrobat Reader available on the computer
- An HTML viewer available on the computer.

Note that these requirements do not depend on the operating system on which the program will be run. DICE can be entirely run from the CD, so there is no special requirement on the disk space. However, the more virtual memory available, the faster the execution time.

The current version of DICE offers two versions of the database. One is a Java, platform independent database that does not require any further drivers. The other one is the OracleLite database, which runs only under the Windows environment. To use this later, the user must install specific drivers.

The master database available on the NEA server can also be accessed. For that, a web connection is required (see the section on local and remote databases).

### Installation

To run the users' interface, you need a Java Virtual Machine installed on your computer (version 1.2 or higher). If Java is already installed (e.g. you had already a previous version of DICE running on your computer), please skip this step. Otherwise, the CD provides two executables (directory dice/java) for Windows and Linux:

- double-click on the file "dice/java/j2re-1\_4\_2-windows-i586.exe" to install the Java runtime on Windows
- execute the file "dice/java/j2re-1\_4\_2-linux-i586-rpm.bin" to install the Java runtime on Linux.

Java runtimes for other operating systems can be obtained on the vendor's web site or on the Java web site (www.java.sun.com).

The installation of Java constitutes the minimum requirement for running DICE. You can already run the interface from the CD and access the Mckoi Java database available on the CD as well. The first version of DICE came with an OracleLite database that can be used on the Windows operating system. To use this database, you need to install some drivers on your system's directory. If you were using a previous version of DICE, these drivers should already be present. If not, please either copy the files in directory "\Dice\oracle\bin" to your computer's system directory (e.g. "C:\Winnt\system32") or use the Oracle\_Lite\_Setup.exe file to install them.

Note that the contents of the Mckoi Java database and of the OracleLite database are the same. The two versions were provided for convenience. If the experience with the Java database is satisfactory, it will likely be the only one available in future versions.

Although not necessary, DICE would run better if the software and the database are installed on a hard drive (or a network drive). This would require about 150 Mbytes. To do so, copy the contents of directory DICE on your drive while keeping the same sub-directories structure. Note that it is not necessary to install the entire handbook (pdf files). DICE can access these pdf files from the CD-ROM.

## **Running DICE**

To run DICE, either from the CD-ROM or from a disk drive, execute the file Dice.bat (for Windows) or Dice.sh (for Unix).

## **Troubleshooting**

The execution files ( .bat or .sh) assume that the java command is in the users' command path. If this is not the case, the program will not run. Alternatively, you may change the execution command to specify the complete path to the java executable. For instance, if java is installed on:

C:\Program Files\ Java\j2re1.4.2\bin\java, add this path between double quotation marks before the first word java. The beginning of the command will thus become:

"C:\Program Files\Java\j2re1.4.2\bin\java" -jar software\DICE.jar

DICE runs better with the Java runtime environment version 1.4 (jre-1.4) or higher. If you are using jre-1.2, you may experience some problems with the size of the windows and panels. To check the java version installed on your computer, type the command: java –version in a DOS, UNIX... command window.

If the user experiences other problems with the software or with the database, please report the problem using the following procedure:

- On Windows, open a DOS command window and go to the directory where file "dice.bat" is located. Type dice.bat and copy the error messages generated by the software during the execution. Send these messages to <a href="mailto:nouri@nea.fr">nouri@nea.fr</a> specifying if the version of DICE used is the one originally distributed with the ICSBEP CD-ROM or if the user has downloaded an updated version from the NEA web site. In the latter case, please specify the approximate date of the last update.
- On Unix, execute the file "dice.sh" and copy the error messages generated by the software during the execution. Send these messages to <a href="mailto:nouri@nea.fr">nouri@nea.fr</a> specifying if the version of DICE used is the one originally distributed with the ICSBEP CD-ROM or if the user has downloaded an updated version from the NEA web site. In such case, please specify the approximate date of the last update.

### **Screen resolution**

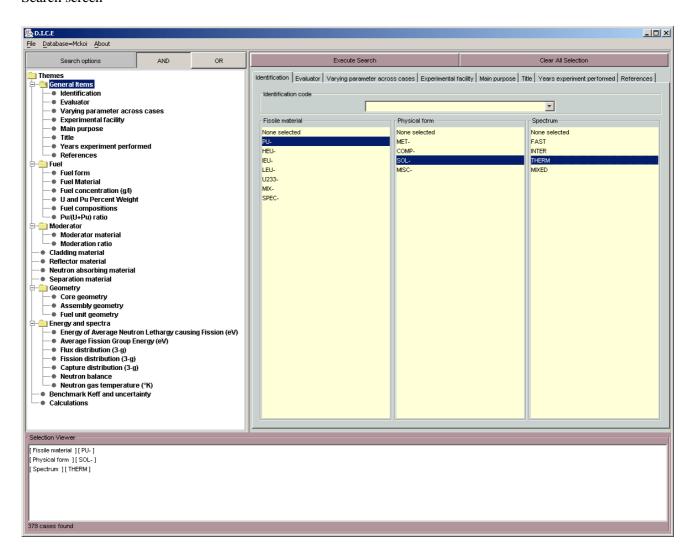
The program automatically adapts the dimensions of its windows to the screen resolution.

## **Using DICE**

#### General overview

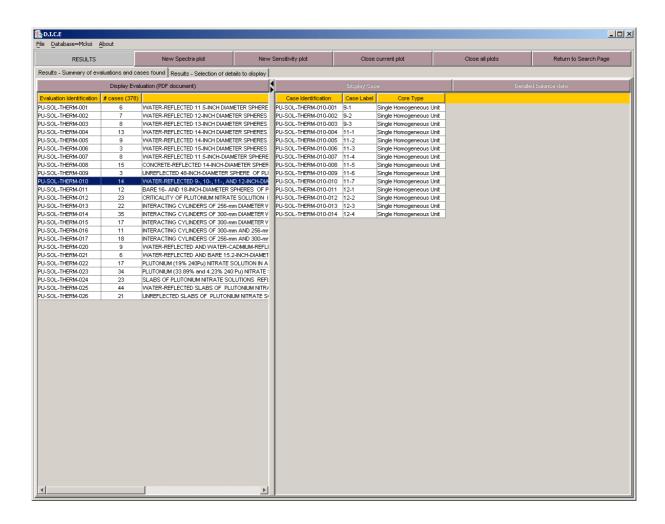
The user's interface is composed of two main screens: "Search screen" and "Results screen". The selection criteria are entered using the "Search screen" and the software interrogates the database for experimental configurations satisfying the selected criteria. Paragraph "Search themes" explains how to enter the selection criteria. A "Selection Viewer" (panel located at the bottom of the screen) gives the list of all specified criteria. This panel is updated when a new criterion is added or when criteria are deleted. To cancel a criterion, the user needs to go back to the corresponding entry in the "Search theme" and select item "None selected". To cancel all criteria, press the button "Clear All Selection".

#### Search screen



#### Results screen

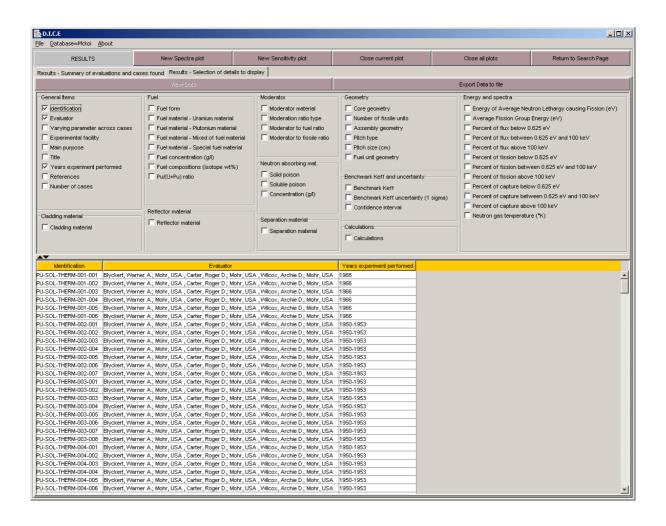
The results page has two panels: the left-hand panel gives the list of evaluations in which an experimental configuration was selected. A column "# cases (NNN)" gives the number of cases in the evaluation which satisfy the criteria. NNN is the total number of cases (sum of numbers in this column). The right-hand panel gives, for each evaluation highlighted in the left-hand panel, the list of cases that satisfy the selection criteria. The complete documentation of the evaluation can be consulted by pressing the button "Display Evaluation (PDF document)". Pressing the button «Display Case» can also generate a summary of each experimental configuration, which gives a concise description of the experiment characteristics (geometry, fuel composition, moderation and reflection conditions, spectra data...).



In addition to the summary pages, the user may want to access specific parameters for all the selected experiments (e.g. variation range of fuel concentration for solutions, moderation to fuel volume ratio in lattices...). This may be useful for parametric analysis of calculation results or for studying correlations between physical parameters. In fact, the "Result screen" contains two tabs located just above the "Display Evaluation (PDF document)" button:

- "Results Summary of evaluations and cases found": lists evaluations and cases meeting the search criteria (previously discussed),
- "Results Selection of details to display" enables the selection of parameters to be displayed in a tabular format (see next screen copy).

When the latter tab is selected, a list of items is displayed from which the user may choose the ones he wants to generate in a tabular format. After selecting the desired parameters and pressing the "View data button", a table is constructed in the lower part of the page. The user may change the order of columns by simple mouse drag and drop. Also, the table may be sorted by ascending order of any of the parameters displayed in the column. The default sorting is ascending order of the first column, which is the experiment identification. To change the sorting order, click on the title of a column and the whole table will be sorted according to the parameter contained in this column. The current version of DICE does not allow plotting graphs of these data. However, the table may be exported into a file using the "Export data to file" button. A dialog window will ask the user to choose the character to be used for separating the values (semicolon, blank...) and for the location and name of the file. The generated tabular file may be used in any graphical package (e.g. MS Excel) to plot graphs.



### Summary table

This table is generated when the button "Display case" is pressed (see above). It summarizes each experimental configuration using the parameters stored in the database. Some of the entries are common to all the configurations contained within the same evaluation (evaluators, publication, and revision dates, title, main purpose of the experimental program, varying parameters across cases, fuel material, name of the laboratory where the experiments were performed, dates the experiments were performed, and the references). Other types of information are specific to one case and concern the description of the geometry, composition, moderation and reflection characteristics, spectra data, benchmark keff and associated uncertainty, and sample calculations. Additional details are given here

for some of these categories. The table is given in html format and can be saved to disk (right click the mouse while selecting the row corresponding to a specific case).

#### **Geometry description:**

To describe the geometry of the experiment, three levels of details were designated.

- 1) *Core geometry:* A description of the overall configuration is given. The possible choices are: Single Homogeneous Unit, Single Assembly, Array of Clad or Unclad Homogeneous Units, Array of Assemblies, or Complex Geometry.
- 2) Assembly description: In the case of configurations containing assemblies, a description is given of the assembly. The possible choices are: Lattice of Fuel Pins or Tubes, Fuel Plates, or Complex Geometry.
- 3) *Basic fuel unit:* Finally the elementary fuel unit is described (pincell in the case of an assembly or the entire unit for homogeneous configurations. The list of choices is much larger in this case.

In the case of complicated shapes for the core or for the assembly, a summary description is given as a free text.

### Composition

The database contains data for fuel compositions. When a configuration contains multiple fissile units of different compositions, all compositions were entered when judged useful (see the discussion below on configurations containing different fissile units). However, some experiments contain several fissile media that differ only slightly. Only a typical or average value is provided on the database. For example, multiple fuel compositions are used in each configuration given in HEU-COMP-INTER-003, but only a typical value is entered into the database.

The data entered into the database are atom densities in atoms/(barn-cm) as given in section 3.3 of the evaluation. However, these data are not displayed in the summary. The data are used, rather, to compute the uranium and plutonium isotopic vectors in weight percents. The atom densities are also used to compute the moderator-to-fuel and the moderator-to-fissile density ratios for homogeneous fuels.

#### Moderator-to-fuel ratio

Depending on the fuel configuration the moderator-to-fuel ratio is calculated as the ratio of atomic densities (homogeneous media) or the ratio of respective volumes (assembly type geometry). For homogeneous media, the moderator-to-fissile atomic densities ratio is also given. For simple cases, this information is automatically calculated from the geometry and composition data. For complex situations, this information was calculated by hand and entered into the database with the mention of the moderation ratio type (atom density or volume ratio...).

#### **Configurations containing different fissile units**

Some experiments contain more than a single type of fissile unit. The difference can be the assembly description (a typical example is reactor experiments with a driver assembly and a test assembly of different pitches), fuel form or composition. For such configurations, the fuel descriptions are entered for the different units and are displayed in the summary.

#### Plotting capabilities

Plotting capabilities were implemented into DICE to allow the user to view graphical representations of neutron spectra such as the flux, reaction rates or sensitivity coefficients. The information used by DICE for the plotting is contained in external text files, i.e. it is not contained within the database.

Once a search is performed, the following buttons appear below the menu bar:

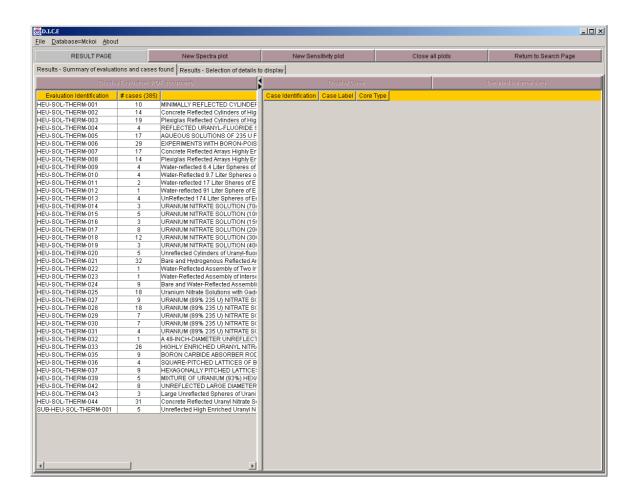
#### **RESULT PAGE**

New Spectra plot

New sensitivity plot

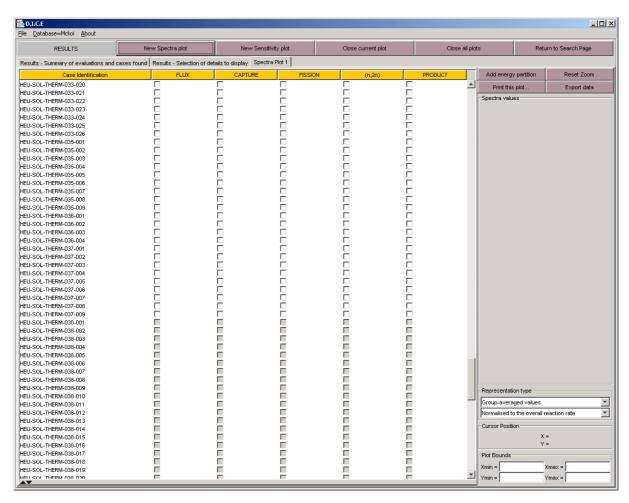
Close all plots

Return to Search Page



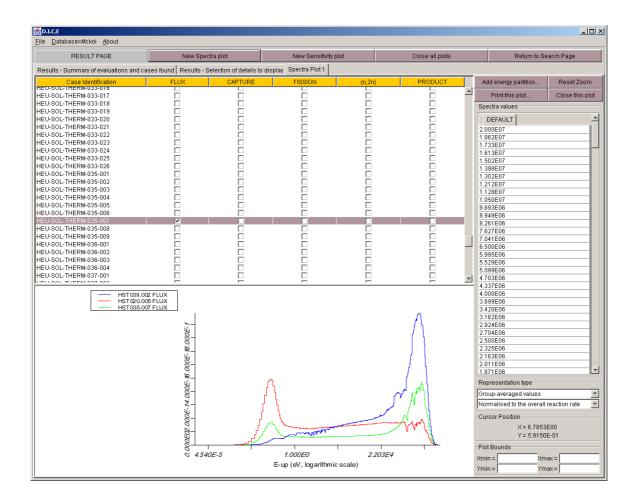
#### How to plot neutron spectra

When pressing the button "New Spectra plot", a new tab is created and is designated as "Spectra Plot 1" (or another number when the "New Spectra plot" button is pressed more than once). The following figure gives a screen capture to illustrate the layout. The panel which appears below the tabs is a table with the identification number of the configurations in the first column followed by columns for the flux, capture, fission, (n,2n) and production reaction rates. In each cell of the table, a selection mark is provided.



Checking one of these marks would generate a plot of the corresponding spectrum (given by the selected column) for the selected configuration (the highlighted line). This is reflected in the legend of each graph (see the figure below). Several selection marks can be checked thus enabling the user to compare the spectra data of various configurations. The gray marks (non-selectable mark) means that the spectra data are not available for this configuration. This can be due to the fact that the spectra data for this configuration was not supplied with this version of DICE. In fact about 10% of the configurations in the 2003 Edition do not have corresponding spectra files. However, if all marks are gray, this means that the software is not looking in the right directory for spectra files. In such case, refer to the "DICE settings" to correct the path to the spectra files.

A feature introduced in the 2003 Edition of DICE allows the user to plot all the fluxes and reaction rates in a selection panel without individually selecting all the marks. If the user is for instance interested in plotting all the fluxes shown in the panel above, then a double click in the yellow cell "Flux" will cause the software to systematically check all the active selection marks in the "Flux" column. To deselect all, simply click on button "Close current plot".



The data used to generate these plots were calculated using the KENO-V.a and KENO-VI codes of the ORNL SCALE code system<sup>1</sup>, the Russian Monte-Carlo code MMK-KENO and ABBN-93 299-energy-group cross section data.

The original flux and reaction rates are given in a 299-group energy mesh (referred to as the DEFAULT mesh). The energy grids are given in the right-hand side panel.

The mouse can be used to zoom to a particular region of the graph. In this case, by using the mouse, the user can simply draw a rectangle in the plotting area, which will define the "[xmin, xmax]" and the "[ymin, ymax]" boundaries. Alternatively, the user can enter specific values for these limits in the "Plot Bounds" frame located at the right-bottom of the screen. The user can at any time come back to the default zoom level (whole energy range and max range for the y-axis) by right clicking with the mouse on the graph or by pressing the button "Reset Zoom" located at the top of the right panel. Other buttons are available in the same panel to print the graph and to close the current graph. On the level just above, other buttons are available to close all graphics, or to create other graphical areas which will be added up as leaflets to be accessed with corresponding tabs.

Several options were implemented to allow the user to customize the graphical display.

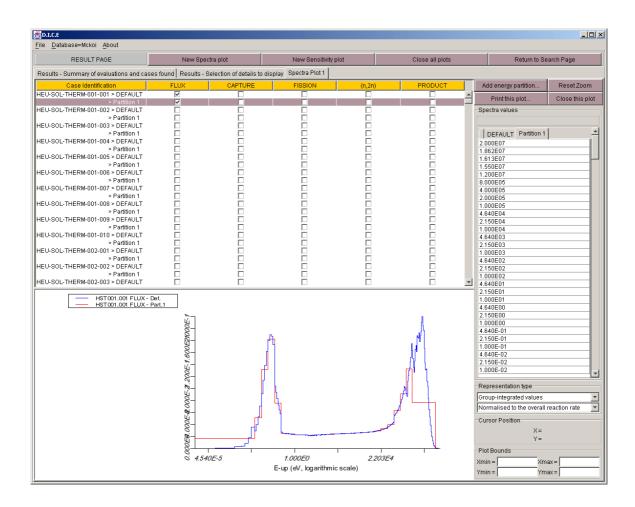
<sup>&</sup>lt;sup>1</sup> RSICC CCC-545 "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, ORNL/NUREG/CSD-2/V2/R5."

#### Changing the energy structure

The user may want to plot the spectra on a broader energy mesh. Starting from the 299-group structure, this might be accomplished by collapsing the information to a broader structure assuming that the reaction rate within each fine group (one of the 299 groups) is constant. While this assumption is valid when each of the broad groups covers several fine groups, the user should keep in mind the underlying approximation, i.e. that the original data is not available in a structure finer than the 299-group.

The button "Add energy partition" located at the top of the right-hand side panel allows the user to browse the computer's disks and directories and choose the name of a text file containing the energy grids of the new energy structure (see DICE Settings options for setting the path to the desired directory). This text file should be structured so that the energies are given by descending order, one energy value per line. Examples are given in directory data/newE.

Once a new energy structure is selected, the selection table is updated with the addition of a new line of selection buttons. For each configuration, the user now has the choice of plotting the spectra in the original energy structure (299-group) designated as "DEFAULT" and in any of the new structures designated as "partition 1", "partition 2". The interface offers the flexibility for plotting any combination of energy structure, reaction rate and configuration. An example is shown in the following screen capture, where the flux in the same configuration is represented in two different energy structures.



#### Choosing the type of representation

The calculated flux and reaction rates contained in the text files and used as primary data for the spectra plotting were defined in that the value in each group is **integrated** over the energy limits of the group. The sum over the whole energy range is equal to 1000 \* the reaction rate, i.e. the data is **normalized** to a **1000 neutrons** emitted in the system.

As the widths of the energy groups in the 299-group structure are not constant, the default option used by DICE is a group-averaged representation (per unit lethargy) instead of a group-integrated representation. The user might change to a group-integrated representation by selecting the appropriate option in the first selection list located at the right-hand side just above the "Cursor Position" frame.

On the other hand, since the magnitude of the flux and of the reaction rates varies from one configuration to the other, the comparison of spectra across configurations may not be simple if they are not normalized to the same value. DICE offers the possibility to change the normalization option from the default option of "Normalised to the overall reaction rate" to the one in which all spectra are normalized to 1.

Note that the two aforementioned choices should be done before the plotting action is activated. Changing the options will not affect the spectra that are already plotted on the graph. In other words, if the user plots a graph with a given choice and wants to change this choice, he has to first deactivate the plot, change his choice of representation and then re-plot.

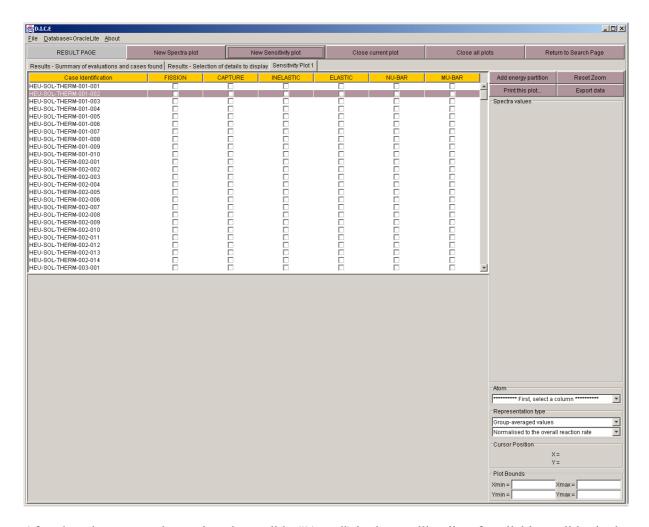
#### How to plot sensitivity coefficients

Sensitivity coefficients are defined as a percent change of the k-eff of a given configuration subject to a one percent change of a particular nuclear data of a certain nuclide in a given energy group. The considered nuclear data processes are: capture, fission, elastic scattering, inelastic scattering, nu-bar (average number of neutron emitted per fission) and mu-bar (average cosine of scattered neutrons). The sensitivity coefficients were calculated using the KEFSF and KEFSFSPH<sup>2</sup> codes on the basis of the transport equation solution by the TWODANT code and the ABBN-93 299-energy-group cross section data.

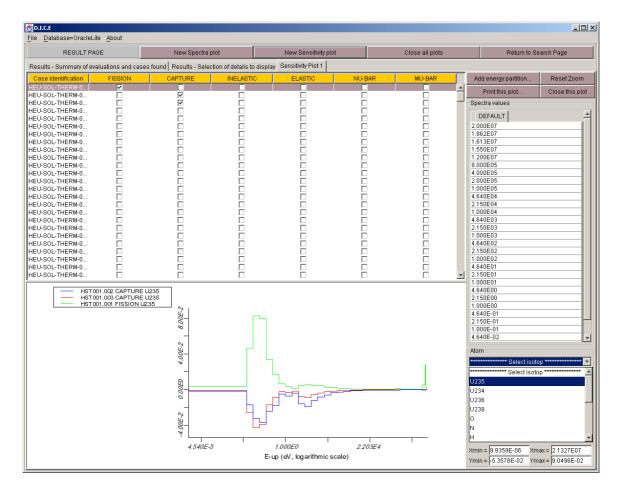
Sensitivity coefficients are currently available in a 30-group energy structure for a selected set of configurations (HEU-SOL-THERM). A directory structure (under data\sensitivity) is used to locate these files (see also the paragraph on DICE Settings). Note that the user might add additional files as they become available and access them through DICE. However, the format of the files should be identical to the format provided on the CD-ROM.

DICE implements an interface to access these files and to plot the sensitivity profiles. A button "New sensitivity plot" is available for this purpose. Once this button is pressed, a table is displayed (see the following screen capture), which allows the selection of the configuration and of the nuclear process.

<sup>&</sup>lt;sup>2</sup> KEFSH and KEFSFSPH are tools developed by IPPE for sensitivity studies. These codes are not yet available in the public domain.



After that, the user needs to select the nuclide ("Atom") in the scrolling list of available nuclides in the composition. The following graph shows examples of such plots.



The options available for the manipulation of the graphs are comparable to those available under the "Spectra plot" feature.

#### Search themes

The search criteria are grouped into several themes. The left-hand panel "Selection Tree" displays the criteria where a theme is symbolized by a folder. Double click on the folder or simple-click on the + sign to expand the folder and to see the criteria included in a theme.

When selecting a theme in the "Selection Tree", the central panel "Selection Panel" displays different tabs, each one corresponding to a search criterion. There is a full correspondence between the "Selection Tree" and the "Selection Panel". To move to a specific criterion within a theme, use either the corresponding tab in the "Selection Panel" or the corresponding bullet in the "Selection Tree".

The selection criteria belong to the following categories. An example will be given for each category.

### Free text

- References
- Title

#### Selection list

- Varying parameters across cases
- Evaluator
- Evaluation identification
- Experimental facility

- Main purpose
- Isotopes present in the fuel composition
- Fuel form
- Fuel material
- Moderator material
- Cladding material
- Reflector material
- Separator material
- Fuel unit geometry (Shape of the)

### Range of integer values

• Years experiment performed

### Range of real values

- Fuel concentration
- Pu/(U+Pu) ratio
- Spectra characteristics (EALF, AFGE, 3-group distributions of flux, fission and capture rates, neutron gas temperature, keff and associated uncertainty)

### Combination of selection list and range of real values

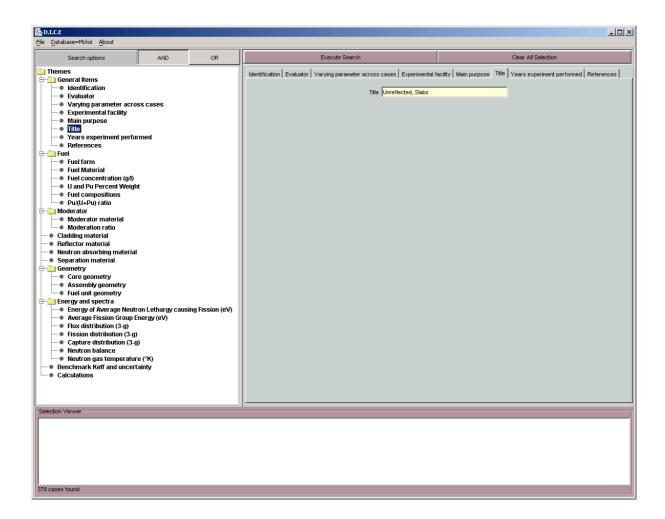
- Core geometry (shape of the core and number of fuel units)
- Moderation ratio (moderation ratio expression –atomic ratio, volume ratio...- and corresponding value)
- Neutron-absorbing material (solid or soluble form and concentration)
- Neutron balance (contribution of a particular isotope to the fission or capture in the core)
- Calculations (results obtained with a combination of code and nuclear data library)
- Assembly geometry description (shape of the assembly, pitch type and value)

Operators "AND" and "OR" can be used to combine *different* selection criteria. For instance, if the user wants to find experiments performed in the sixties containing nitrate uranium fuel, the operator "AND" should be used to combine the criteria on "Years experiments performed" and "Fuel material". Operator "AND" is used by default to combine multiple criteria. However, if the user is interested in experiments where iron is used either as a separator material or as a reflector then operator "OR" should be used to combine the corresponding criteria.

When an elementary selection criterion is composed of several criteria (for instance "U and Pu Percent Weight" contains two separate criteria on uranium and plutonium isotopic vectors), then operator "OR" is implicitly used to combine these criteria. If the user searches for experiments containing more than 90% percent weight of U235 and Pu239, then the result will be a combination of high-enriched uranium systems, plutonium systems and mixed uranium and plutonium systems.

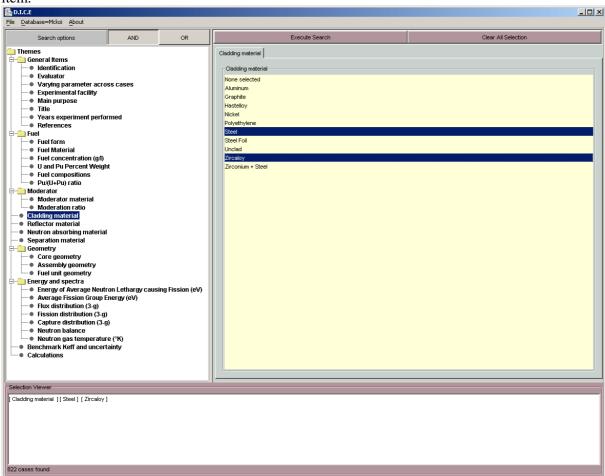
## Example of a free text field selection

Enter one or multiple words separated with a comma and choose between the two options Or/And. The program will search the occurrence of these words according to the specified option.



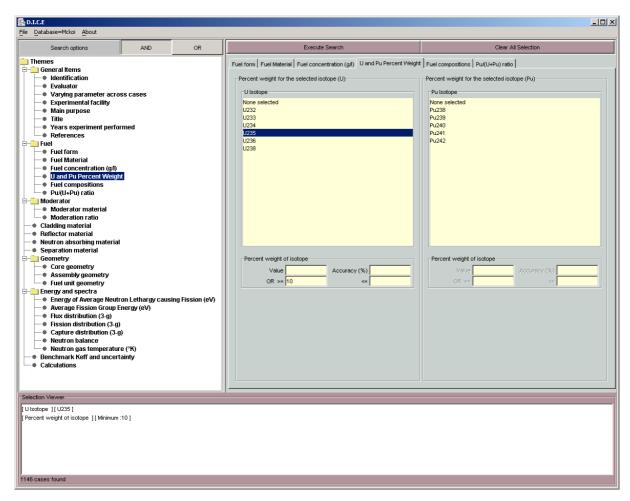
### Example of a selection in a selection list

In all selection lists, the first item is "None selected". This allows canceling a selected item in the list. Multiple selection is possible by maintaining the Shift or Ctrl keys pressed. If several items are selected, and the user needs to cancel one of them, maintain the Ctrl key pressed and re-select this item.



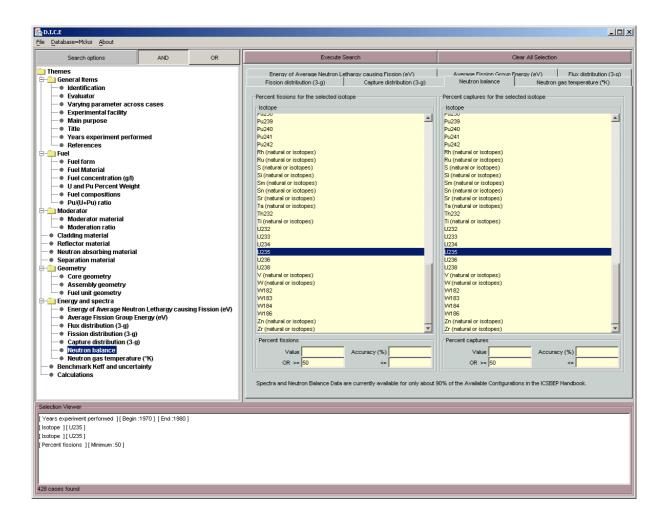
### Example of a selection in range of real values

Specify the parameter value (in the specified units) with a percent accuracy, e.g. 100 with an accuracy of 10% would return values between 90 and 110. Alternatively, the range can explicitly be entered (minimum and maximum values). The inequalities are not strict.



Example of a selection in a combination of selection list and range of real values

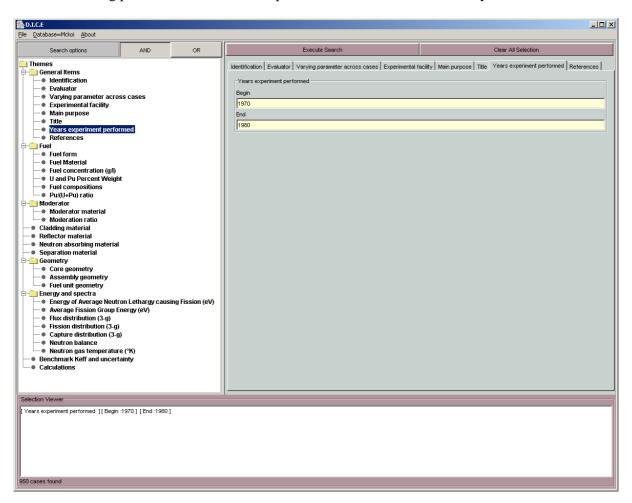
For some search criteria, there is correspondence between the selection list and the range of entered values. This means that this range will be applied to the specific item selected in the list. In the following example, a search will be made for experiments in which the U-235 contribution to fission and capture are higher than 50%.



Example of a selection in a range of integer values

"Years experiments performed" is the only one in this category. For example, one may search experiments performed in the eighties (1980-1989). In this case, experimental programs started before 1980 but ended after 1980 will be counted as well. One can also search for experiments performed before (or after) a certain year. The specified years (minimum and maximum are counted).

Note: For a few experimental programs, there was a discontinuity in the operation. For instance, experiment HEU-MET-FAST-008 was performed in 1982 and in 1995. They are treated in the database as being performed over the whole period of time without discontinuity.



#### Local and remote databases

The CD-ROM provides two versions of local databases in directory Dice\databases. The first is Mckoi, a Java database which should run on almost all platforms, and the second is the OracleLite database to be used on Windows. The contents of these databases are the same, and they reflect the status of data entries at the date of publication.

The central database is located on the NEA web site where corrections and additions are implemented as needed. This database is to be utilized if the user wishes to access the latest version of the data entries. The connection is made through the Java Remote Method Invocation technique and does not require any extra driver or software on the user's computer, except for a web connection.

The menu "database" enables the user to switch from one version to the other by choosing one of the following options: "Mckoi", "Oracle" and "NEA". The default database at the start-up is "Mckoi".

#### Live update

Changes will continue to be made to the software and to the database after the publication of the CD-ROM. A live-update option enables the user who has a web connection to automatically check the updates and download the necessary files from the NEA website. However, as this option replaces the old versions of the files, they should not have a read-only status. Thus, running this option requires the software and the database to be installed on a hard drive with a "write" permission.

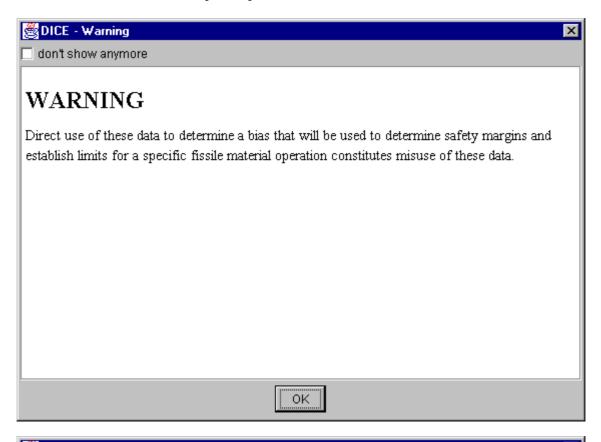
This option is not activated by default. To run the live-update at each start-up or at regular time intervals, see the next paragraph (settings) for details. To run the live-update instantaneously, choose the menu option "File/check update...". Each time a new version of the software or of the database is available on the NEA web, the program downloads it and replaces the old version. The old version is not deleted but rather renamed. The user is advised to clean-up his "software" and "database" directories after an update by deleting files named "dice.odb.bckdate\_and\_time" and "DICE.jar.bckDate\_and\_time".

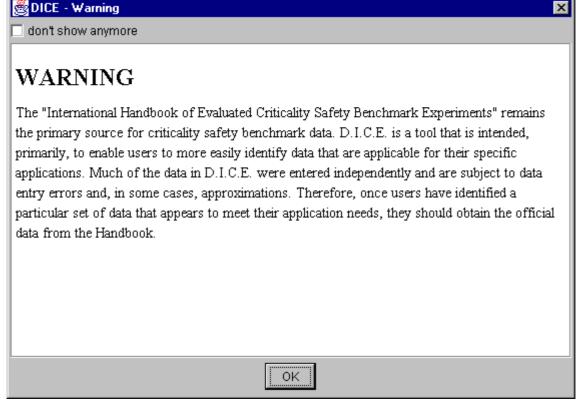
#### **Settings**

Different default options can be changed using the menu "File/Settings". This enables the user to specify:

- The directory where the pdf files of the ICSBEP handbook are located. The default directory is Cd2003 located at the same level as the dice.bat file.
- The path to the Acrobat Reader viewer. The default viewer is automatically launched on Windows. For other operating systems or if the user wishes to launch a different version of Acrobat, the complete path to the viewer should be specified.
- The path to the HTML browser. As for the pdf viewer, the default browser is automatically launched on Windows. For other operating systems or if the user wishes to launch a different browser to view the summary tables, the complete path to the browser should be specified.
- The name of the directory where the detailed spectra data files are stored. This directory contains sub-directories named after the fuel type (e;g. PU, HEU, LEU...), and the actual file names are of type HST001.001, i.e. a representation of the configuration name.
- The path to files describing energy schemes.
- The name of the directory where the sensitivity files are stored. This directory contains subdirectories named after the fuel type (e;g. PU, HEU, LEU...) and the actual file names are of type HST001.001, i.e. a representation of the configuration name.
- The name of the directory where the detailed balance data are stored.
- The path to the desired text file editor to be used when opening the detailed balance data files. If nothing is specified, the default Java text editor is used.

- The display of the warning pop-up windows (see below) at startup and at results export. Note that both pop-up windows have an option for deactivating their display (checkbox on the top left of the pop-up windows).
- The activation of the Live-update option.





## **Contributors**

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